



Stability of Nanoscale Surficial Films on Silicon*

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Goal: It has been shown that intergranular films in silicon nitride and surficial bismuth oxide films on zinc oxide achieve stability at thicknesses of a few monolayers. The goal of this research is to determine whether doped and undoped surficial films on silicon exhibit stability at thicknesses as low as a partial monolayer. Figure 1 on the right illustrates the typical behavior of Si_3N_4 and $\text{ZnO-Bi}_2\text{O}_3$ film coverage as a function of adsorbate activity (black curves). A predicted behavior for our Si/SiO_x system is plotted in blue.

Impact: Surficial and intergranular films in silicon are the basis of microelectronic and future nanoelectronic devices. Understanding how to analyze these films will have direct scientific impact.

Preliminary Results: Samples were prepared using a Zr/ZrO_2 buffer to fix the oxygen activity in the system during heat treatment. Angle resolved X-ray Photoelectron Spectroscopy (XPS) measurements were then performed to compare the thickness of these films with those of films annealed under the same conditions in the absence of the buffer. Figure 2 shows the respective Si 2p peaks measured at 70° detection angle (shallow photoelectron escape depth). The sample annealed with the Zr/ZrO_2 buffer (a) is very slightly, substoichiometrically oxidized whereas the unbuffered sample (b) contains a significant SiO_2 peak at 104 eV. These results suggest that partial monolayer thick films may be stable on silicon when processed in the presence of a metal/metal oxide buffer.

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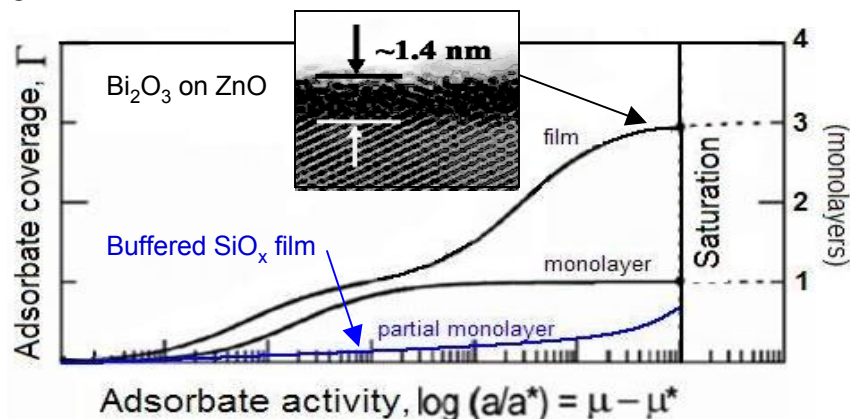


Figure 1. Predicted wetting behavior of the buffered Si/SiO_x system (blue curve) as compared to that of previously studied Si_3N_4 and Bi_2O_3 films.

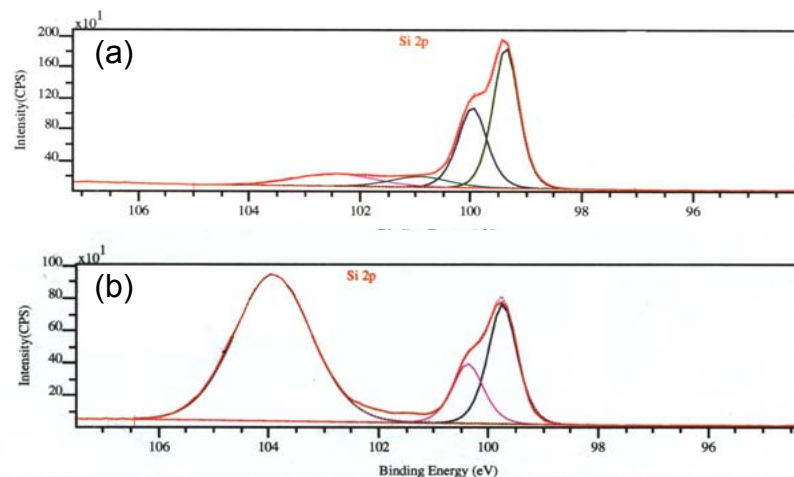


Figure 2. Si 2p XPS peaks of SiO_x films annealed in a Zr/ZrO_2 buffered system (a), and in the absence of buffer (b).



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Education and Collaboration:

Undergraduate Ana Ramos is currently working on this project at MIT with Ph.D. student Ming Tang. As part of the NSF-EC NANOAM collaboration, she traveled to the CEA-Saclay laboratory in France this summer where she spent three months doing research with NANOAM P.I. Martine Gautier-Soyer. Throughout the summer, samples and results were exchanged between both laboratories and results were presented in July at the NANOAM midterm conference in Karlsruhe, Germany. Ana is also actively involved in the MIT International Science and Technology Initiatives (MISTI) program, and her work in France has served as a model for current research collaborations between MIT and France.



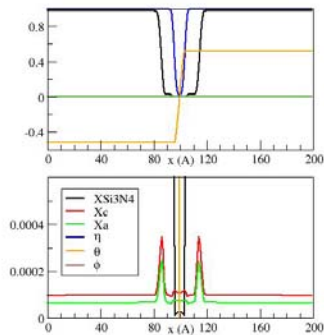
Ana Ramos (far right) speaking to the MIT-France Advisory board about her NANOAM research in France. Pictured second from the left is the French Ambassador to the US, H.E. Jean-David Levitte.

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Nanometer Scale Induced Structure between Amorphous Layers and Crystalline Materials

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Phase-field modeling that coarse-grains small-scale physics is used to simulate intergranular films in silicon nitride. An example of a stabilized film with structure and chemistry not found in bulk equilibrium is presented at left.

The films are also being examined as confined liquids using classical liquid density functional theory. Well developed theory is applied to investigate the dominant effects for stabilizing ordered structures in simple systems.



As part of the EU/NSF partnership on this project, Catherine Bishop is a post-doc at Oxford University. Her work is bridging the gap between ab-initio calculations and thermodynamic modeling



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